Table D3. Individual hydrocarbon and total petroleum hydrocarbon concentrations (in μg/g wet wt.) for sediment cores taken from the Mill Creek marsh, a reference site.[1-4]

Sample ID	Core Section No[5]	Nonane ($n\text{-}C_9$)	Decane ($n\text{-}C_{10}$)	Undecane ($n\text{-}C_{11}$)	Dodecane ($n\text{-}C_{12}$)	Tridecane ($n\text{-}C_{13}$)	Tetradecane ($n\text{-}C_{14}$)	Pentadecane ($n\text{-}C_{15}$)	Hexadecane ($n\text{-}C_{16}$)	Heptadecane ($n\text{-}C_{17}$)	Pristane	Octadecane ($n\text{-}C_{18}$)	Phytane	Nonadecane ($n\text{-}C_{19}$)	Eicosane ($n\text{-}C_{20}$)	Heneicosane ($n\text{-}C_{21}$)	Docosane ($n\text{-}C_{22}$)	Tricosane ($n\text{-}C_{23}$)
Station A[6]																		
1098032311	1	nd	nd	nd	nd	nd	nd	nd	nd	2.11	nd	nd	nd	nd	nd	nd	nd	nd
1098032312	2	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
1098032313	3	nd	nd	nd	nd	nd	nd	nd	nd	nd	1.57	nd	2.11	nd	nd	nd	nd	nd
1098032314	4	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
Whole Core: Average[7,8]		nd	nd	nd	nd	nd	nd	nd	nd	< MDL	< MDL	nd	< MDL	nd	nd	nd	nd	nd
Whole Core: Std. Dev.		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Station B																		
1098032306	1	nd	nd	nd	nd	nd	nd	nd	nd	2.24	nd	nd	nd	3.21	nd	nd	nd	nd
1098032307	2	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
1098032308	3	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
1098032309	4	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	1.53	nd	nd	nd	nd
1098032310	5	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
Whole Core: Average[7,8]		nd	nd	nd	nd	nd	nd	nd	nd	< MDL	nd	nd	nd	1.34	nd	nd	nd	nd
Whole Core: Std. Dev.		-	-	-	-	-	-	-	-	-	-	-	-	1.12	-	-	-	-
Station C																		
1098032301	1	nd	nd	nd	nd	nd	nd	nd	nd	1.73	nd	nd	nd	nd	nd	nd	nd	nd
1098032302	2	nd	nd	nd	nd	nd	nd	nd	nd	2.24	nd	nd	nd	2.13	nd	nd	nd	nd
1098032303	3	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
1098032304	4	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
1098032305	5	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
Whole Core: Average[7,8]		nd	nd	nd	nd	nd	nd	nd	nd	< MDL	nd	nd	nd	< MDL	nd	nd	nd	nd
Whole Core: Std. Dev.		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Station D																		
1098032316	1	nd	nd	nd	nd	nd	nd	nd	nd	2.03	nd	nd	nd	nd	nd	nd	nd	nd
1098032317	2	nd	nd	nd	nd	nd	nd	nd	nd	2.52	nd	nd	nd	nd	nd	nd	nd	nd
1098032318	3	nd	nd	nd	nd	4.89	4.58	11.5	2.97	11.4	13.2	8.42	8.29	8.65	3.68	4.06	nd	nd
1098032319	4	nd	nd	2.56	3.06	5.08	19.6	nd	5.68	7.66	6.92	nd	nd	6.04	nd	nd	3.42	nd
1098032320	5	nd	8.66	nd	3.53	3.37	18.2	8.06	8.23	8.64	10.4	nd	3.16	1.58	1.37	nd	nd	nd
Whole Core: Average[7,8]		nd	2.53	< MDL	< MDL	3.06	8.87	4.43	3.68	6.45	6.37	2.23	2.68	3.51	1.41	< MDL	< MDL	nd
Whole Core: Std. Dev.		-	3.43	-	-	2.01	9.29	5.03	3.25	4.06	5.65	3.46	3.32	3.64	1.30	-	-	-
MDL		2.57	1.99	2.09	2.03	1.97	1.98	1.73	1.53	1.48	1.35	1.37	1.29	1.30	1.34	1.44	2.52	1.84

Table D3. Continued.[1-3]

Sample ID	Core Section No[5]	Tetracosane (n-C_{24})	Pentacosane (n-C_{25})	Hexacosane (n-C_{26})	Heptacosane (n-C_{27})	Octacosane (n-C_{28})	Nonacosane (n-C_{29})	Triacontane (n-C_{30})	n-Hentriacontane (n-C_{31})	Dotriacontane (n-C_{32})	Tritriacontane (n-C_{33})	Tetratriacontane (n-C_{34})	Pentatriacontane (n-C_{35})	Hexatriacontane (n-C_{36})	Heptatriacontane (n-C_{37})	Octatriacontane (n-C_{38})	Nonatriacontane (n-C_{39})	Tetracontane (n-C_{40})
Station A[6]																		
1098032311	1	nd	nd	nd	nd	nd	3.66	nd	7.61	nd	17.9	nd	nd	nd	nd	nd	nd	nd
1098032312	2	nd	nd	nd	nd	nd	3.90	nd	7.02	nd	nd	nd	nd	nd	nd	nd	nd	nd
1098032313	3	nd	nd	nd	nd	nd	nd	nd	5.26	nd	20.2	nd	nd	1.52	nd	nd	nd	nd
1098032314	4	nd	nd	nd	nd	nd	3.56	nd	6.29	nd	nd	nd	nd	1.91	nd	nd	nd	nd
Whole Core: Average[7,8]		nd	nd	nd	nd	nd	3.17	nd	6.54	nd	11.6	nd	nd	1.04	nd	nd	nd	nd
Whole Core: Std. Dev.		-	-	-	-	-	1.08	-	1.01	-	8.67	-	-	0.80	-	-	-	-
Station B																		
1098032306	1	nd	nd	nd	nd	nd	3.47	nd	8.38	nd	17.1	nd	nd	nd	nd	nd	nd	nd
1098032307	2	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
1098032308	3	nd	nd	nd	nd	nd	3.56	nd	7.45	nd	12.7	nd	nd	0.91	nd	nd	nd	nd
1098032309	4	nd	nd	nd	nd	nd	nd	nd	5.68	nd	32.0	nd	nd	1.92	nd	nd	nd	nd
1098032310	5	nd	nd	nd	nd	nd	nd	nd	5.73	nd	42.4	nd	nd	1.42	nd	nd	nd	nd
Whole Core: Average[7,8]		nd	nd	nd	nd	nd	< MDL	nd	5.65	nd	21.7	nd	nd	1.00	nd	nd	nd	nd
Whole Core: Std. Dev.		-	-	-	-	-	-	-	2.84	-	15.4	-	-	0.68	-	-	-	-
Station C																		
1098032301	1	nd	nd	nd	nd	nd	nd	nd	8.18	nd	18.2	nd	nd	nd	nd	nd	nd	nd
1098032302	2	nd	nd	nd	nd	nd	3.61	nd	8.02	1.89	17.6	nd	nd	nd	nd	nd	nd	nd
1098032303	3	nd	nd	nd	nd	nd	4.85	nd	8.03	2.21	nd	nd	nd	0.90	nd	nd	nd	nd
1098032304	4	nd	nd	nd	nd	nd	5.27	nd	7.23	2.31	40.7	nd	nd	0.94	nd	nd	nd	nd
1098032305	5	nd	nd	nd	nd	nd	4.18	nd	7.66	1.95	nd	nd	nd	1.07	nd	nd	nd	nd
Whole Core: Average[7,8]		nd	nd	nd	nd	nd	3.90	nd	7.82	1.83	17.0	nd	nd	< MDL	nd	nd	nd	nd
Whole Core: Std. Dev.		-	-	-	-	-	1.45	-	0.38	0.60	15.0	-	-	-	-	-	-	-
Station D																		
1098032316	1	nd	nd	nd	nd	nd	3.29	nd	8.66	2.51	10.3	nd	nd	nd	nd	nd	nd	nd
1098032317	2	nd	nd	nd	nd	1.63	3.54	1.65	5.42	2.02	nd	0.74	nd	nd	nd	nd	nd	nd
1098032318	3	nd	nd	1.62	nd	3.04	4.42	3.75	3.05	nd	nd	nd	nd	nd	nd	nd	nd	nd
1098032319	4	nd	nd	1.89	2.03	1.74	3.98	2.77	2.57	nd	nd	0.74	nd	nd	nd	nd	nd	nd
1098032320	5	nd	2.13	nd	nd	3.43	3.81	nd	3.01	nd	nd	nd	nd	nd	nd	nd	nd	nd
Whole Core: Average[7,8]		nd	< MDL	< MDL	< MDL	2.12	3.81	1.85	4.54	< MDL	< MDL	< MDL	nd	nd	nd	nd	nd	nd
Whole Core: Std. Dev.		-	-	-	-	1.10	0.43	1.42	2.56	-	-	-	-	-	-	-	-	-
MDL		1.47	1.69	1.39	1.96	1.51	3.13	1.05	2.03	1.60	8.25	0.71	1.25	0.73	0.68	0.61	0.53	0.56

Table D3. Continued.[1-3]

Sample ID	Core Section No[5]	Total Petroleum Hydrocarbons[9]	Total Concentrations of Individual Hydrocarbons[10,11,19]	Total: Pristane + Phytane[10,19]	Pristane/n-C_{17}[20]	Phytane/n-C_{18}[20]	Pristane/Phytane[20]	Total: Odd No Carbons[10,12,19]	Total: Even No Carbons[10,13,19]	Carbon Preference Index (CPI)[14,20]	Sum: C_{10}-C_{12}-C_{14}[10,15,19]	Sum: C_{22}-C_{24}-C_{26}-C_{28}[10,16,19]	Weathering Index (WI)[17,20]
Station A[6]													
1098032311	1	nd	nd	nd	-	-	-	40.8	nd	-	nd	nd	-
1098032312	2	nd	nd	nd	-	-	-	nd	nd	-	nd	nd	-
1098032313	3	nd	nd	3.69	-	-	0.75	37.3	nd	-	nd	nd	-
1098032314	4	nd	nd	nd	-	-	-	nd	nd	-	nd	nd	-
Whole Core: Average[7,8]		nd	nd	< MDL	-	-	-	< MDL	nd	-	nd	nd	-
Whole Core: Std. Dev.		-	-	-	-	-	-	-	-	-	-	-	-
Station B													
1098032306	1	nd	nd	nd	-	-	-	43.3	nd	-	nd	nd	-
1098032307	2	nd	nd	nd	-	-	-	nd	nd	-	nd	nd	-
1098032308	3	nd	nd	nd	-	-	-	34.0	nd	-	nd	nd	-
1098032309	4	nd	64.5	nd	-	-	-	50.4	nd	-	nd	nd	-
1098032310	5	nd	73.5	nd	-	-	-	59.9	nd	-	nd	nd	-
Whole Core: Average[7,8]		nd	< MDL	nd	-	-	-	40.9	nd	-	nd	nd	-
Whole Core: Std. Dev.		-	-	-	-	-	-	16.4	-	-	-	-	-
Station C													
1098032301	1	nd	nd	nd	-	-	-	39.2	nd	-	nd	nd	-
1098032302	2	nd	nd	nd	-	-	-	42.5	nd	-	nd	nd	-
1098032303	3	nd	nd	nd	-	-	-	nd	nd	-	nd	nd	-
1098032304	4	nd	78.1	nd	-	-	-	63.5	nd	-	nd	nd	-
1098032305	5	nd	nd	nd	-	-	-	nd	nd	-	nd	nd	-
Whole Core: Average[7,8]		nd	< MDL	nd	-	-	-	35.8	nd	-	nd	nd	-
Whole Core: Std. Dev.		-	-	-	-	-	-	19.6	-	-	-	-	-
Station D													
1098032316	1	nd	nd	nd	-	-	-	nd	nd	-	nd	nd	-
1098032317	2	210	nd	nd	-	-	-	nd	nd	-	nd	nd	-
1098032318	3	2540	114	21.5	1.16	0.98	1.59	58.4	34.2	1.71	6.59	nd	-
1098032319	4	1660	91.2	7.56	0.90	-	-	39.9	43.7	0.91	23.6	7.79	3.04
1098032320	5	2070	104	13.5	1.20	-	3.29	40.9	49.4	0.83	30.4	nd	-
Whole Core: Average[7,8]		1310	73.6	9.04	0.99[21]	1.20[21]	2.38[21]	34.6	29.9	-	13.3	< MDL	2.25[21]
Whole Core: Std. Dev.		1110	41.1	8.61	-	-	-	17.7	18.0	-	12.8	-	-
MDL		181	59.0[18]	2.63[18]				33.9[18]	22.4[18]		5.99[18]	6.89[18]	

Table D3. Continued.

Footnotes:

[1] No surface skim samples were analyzed for Mill Creek Marsh.

[2] The concentrations of the individual aliphatic hydrocarbons and the total petroleum hydrocarbons were determined using external standard calculations.

[3] When an individual aliphatic hydrocarbon was not detected, its concentration was replaced by nd.

[4] The concentrations for n-C_8 will be not reported, since it was difficult to identify this peak in samples and to determine MDL for n-C_8. A value of 0 was used for each nondetected analyte in summation formulae.

[5] For the sediment cores, these numbers represent the depths into each core: 1 - depth 0 to 1 cm; 2 - depth 1 to 2 cm; 3 - depth 2 to 3 cm; 4 - depth 3 to 4 cm; and, 5 - depth 4 to 5 cm.

[6] The extract for core section 5 for Station A was lost during sample cleanup.

[7] The Whole Core Average and Standard Deviation is calculated using the concentrations for each analyte over all core sections.

[8] If all concentrations are nd, the average is replaced with nd. When there is at least one number in the data set to be averaged, each nd is replaced with 1/2*MDL, and an average is calculated. If this numeric value is less than the MDL, the average is replaced by < MDL; otherwise, the average is the calculated value. When a numeric value is found for the average, the standard deviation is then determined using the same number set used to calculate the average.

[9] Determined from the total peak areas in the chromatogram from n-C_8 to n-C_{40} minus any contributions from the internal standard areas.

[10] These formulae use 1/2MDL values for each analyte not detected.

[11] Sum of the concentrations of the individual aliphatic hydrocarbons n-C_9 through n-C_{40} plus the concentrations of pristane and phytane.

[12] The total of the concentrations of the aliphatic hydrocarbons with an odd number of carbon atoms.

[13] The total of the concentrations of the aliphatic hydrocarbons with an even number of carbon atoms. The contribution of n-C_8 is not included in the total.

[14] Carbon Preference Index (CPI) defined as the ratio of the total of the concentrations of the aliphatic hydrocarbons with an odd number of carbons to the total concentration of the alphatic hydrocarbons with an even carbon number.

[15] The total of the concentrations of n-C_{10}, n-C_{12}, and n-C_{14}.

[16] The total of the concentrations of n-C_{22}, n-C_{24}, n-C_{26}, and n-C_{28}.

[17] Weathering Index (WI) is defined as the ratio of the total concentration of n-C_{10}, n-C_{12}, and n-C_{14} to the total concentration of n-C_{22}, n-C_{24}, n-C_{26}, and n-C_{28}.

[18] These MDL values are calculated with the same summation formulae as the samples using the individual hydrocarbon MDL values.

[19] The summation totals for the samples are compared with calculated MDL values obtained using the same summation formulae as the samples. When these sample totals were less than the total MDL, its value was replaced by nd. The averages and standard deviations for the totals were treated in the same way as the individual hydrocarbons; see footnote 8.

[20] Numerical values of the CPI, WI, and the ratios: pristane/n-C_{17}, phytane/n-C_{18}, and pristane/phytane, will be calculated only when the defined quantity for each index or ratio has a numeric value.

[21] These results are not true averages, instead they are the ratios of the averages of the defined quantities, if these averages exist.